# Quantum discord in spin systems with dipole-dipole interaction

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The behavior of total purely quantum correlation (discord) in dimers consisting of dipolar-coupled spins 1/2 is studied. We found that the discord Q = 0 at the absolute zero temperature. With increasing the temperature T, at first the quantum correlations in the system increase, smoothly reach the maximum, and then turn again into zero according to the asymptotic law  $T^{-2}$ . It is also shown that in absence of external magnetic field B, the classical correlation C at  $T \to 0$  is, vice versa, maximal. Our calculations predict that in crystalline gypsum CaSO<sub>4</sub> · 2H<sub>2</sub>O the value of natural (B = 0) quantum discord between nuclear spins of hydrogen atoms is maximal at the temperature of 0.644  $\mu$ K, and for 1,2-dichloroethane H<sub>2</sub>ClC - CH<sub>2</sub>Cl the discord achieves the largest value at  $T = 0.517 \ \mu$ K. In both cases, the discord equals  $Q \approx 0.083$  bit/dimer what is 8.3% of its upper limit in two-qubit systems. We estimate also that for gypsum at room temperature  $Q \sim 10^{-18}$  bit/dimer, and for 1,2-dichloroethane at T = 90 K the discord is  $Q \sim 10^{-17}$  bit per a dimer.

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# I. INTRODUCTION

The notion quantum discord has been introduced in the quantum information theory by Zurek<sup>1</sup>. Discord was regarded as "a measure of a violation of classicality of a joint state of two quantum subsystems"<sup>1</sup>. However later its initial definition undergone some changes.

In 2001, Henderson and Vedral and then independent of them Ollivier and Zurek in their papers<sup>2,3</sup> (see  $also^{4,5}$ ) performed analysis of every possible correlations I in a bipartite system and suggested the ways to extract from them, on the one hand, the purely classical part Cand, on the other hand, only the quantum contribution Q. The quantum excess of correlations, Q = I - C, has been called "discord" in the modern understanding of this term<sup>3</sup>.

The authors of above papers established also that the quantum correlation can be non-zero even in separable (but mixed) states. In other words, quantum correlations are not exhausted by entanglement (E). Entanglement, which can relate the different parts of a system even when there are no interactions between these parts (the Einstein-Podolsky-Rosen effect), is only a special kind of quantum correlations. Since the 80–90s of past century the entanglement was considered as a fundamental resource for quantum information processing, teleportation, cryptography, metrology, and other tasks in quantum technology<sup>6–10</sup>.

It is remarkable that quantum discord can also lead to a speedup over classical computation and lead even without containing much entanglement<sup>11,12</sup>. This important property of discord evoked extremely great interest to the new kind of correlations. One discovered also that discord can detect the quantum phase transitions<sup>13,14</sup>. Moreover, it has been shown that in contrast to entanglement and thermodynamical quantities, the discord makes it possible to catch the approach of quantum phase transitions even at finite temperatures<sup>15</sup>. Other important features of discord have been also noted. By this, a surprising fact turned out: "Almost all quantum states have nonclassical correlations"<sup>16</sup>. Achieved up to now results on the theory and applications of quantum discord are given in the recent reviews<sup>17,18</sup>.

The goal of this paper is to study the behavior of discord in spin systems with dipolar couplings. There is a large number of substances magnetic interactions in which have the dipole-dipole character, and exchange and indirect ones are weak enough. By this, the spins both electrons and nuclears can serve as elementary magnetic moments. The class of dipolar magnets with electron spins includes, for example, the Tutton salts, alums<sup>19</sup>, and numerous salts of rare earth elements<sup>20</sup>. The typical temperatures at which the effects of their dipole interactions show themselves lie in the millikelvin region. However the spin-lattice interactions in electron paramagnets are strong that leads to short relaxation times too. Nuclear spins, of course, have an indubitable asset: the spin-lattice relaxation times for them can achieve minutes and hours. Using the available NMR data for the two classical examples, gypsum  $CaSO_4 \cdot 2H_2O^{21}$  and 1,2-dichloroethane  $H_2ClC - CH_2Cl^{22}$  (see also, e.g.,<sup>23,24</sup>) which contain the sufficiently isolated pairs of dipolarcoupled nuclear hydrogen spins, we estimate

In following sections of the paper we give definitions for the different correlations, formulate the model, calculate the classical and quantum information correlations in it, estimate the discord for materials with spin-nuclear dimers, and, lastly, briefly summarize the results obtained.

# II. CLASSICAL AND QUANTUM CORRELATIONS

In statistical theory, a degree of relationship (correlation) between two random variables xand y with the joint probability distribution function p(x, y) is often measured by covariations or by Pearson's correlation coefficient

$$R = \frac{\overline{(x - \overline{x})(y - \overline{y})}}{\sqrt{D_1}\sqrt{D_2}}.$$
 (1)

Here the bar denotes the average over the probability distribution and  $D_1 = (x - \overline{x})^2$  and  $D_2 = \overline{(y - \overline{y})^2}$  are dispersions respectively for xand y. Notice that in the mathematical statistics other types of correlation coefficients are used also. One should emphasize that the condition R = 0 does not imply, generally speaking, the independence of random variables, i. e., that  $p(x, y) = p_1(x)p_2(y)^{25,26}$ .

In the classical information theory (e.  $g.,^{27,28}$ ), one uses the notion of mutual information

$$I(X:Y) = H(X) + H(Y) - H(X,Y) \ge 0 (2)$$

between two objects X Y. Here H(X), H(Y), and H(X,Y) are the Shannon entropies

$$H(X) = -\sum_{x} p_{1}(x) \log p_{1}(x),$$
  

$$H(Y) = -\sum_{y} p_{2}(y) \log p_{2}(y),$$
  

$$H(X,Y) = -\sum_{x,y} p(x,y) \log p(x,y), \quad (3)$$

where  $p_1(x) = \sum_y p(x, y)$ ,  $p_2(y) = \sum_x p(x, y)$ . (A choose of logarithm base defines the information measure unities: bits, nats, dits, hartley.) It is remarkable that now the equality I = 0 is a necessary and sufficient condition for the independence of X and Y. This property allows to use the mutual information as a measure of information correlation between the systems X and  $Y^{25}$ . Taking into account the Bayes rule one can rewrite the right part of Eq. (2) in Shannon's nonsymmetric form

$$I'(X:Y) = H(X) - H(X|Y),$$
(4)

where

$$H(X|Y) = H(X,Y) - H(Y)$$
(5)

is the condition entropy. In the classical case,  $I' \equiv I$ .

In the quantum information theory<sup>6,29</sup>, the equation (2) is replaced by the new definition

$$I(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \quad (6)$$

which serves as a measure of quantum mutual information between the two subsystems A and B composing together the joint system AB = $A \cup B$ . In Eq. (6),  $\rho_{AB}$  is the density matrix of the joint system AB,  $\rho_A$  and  $\rho_B$  are the reduced density matrices, respectively, for subsystems A and B, and  $S(\rho)$  ( $\rho = \{\rho_A, \rho_B, \rho_{AB}\}$ ) represents the von Neumann entropy

$$S(\rho) = -\operatorname{Tr} \rho \log \rho. \tag{7}$$

It is important that I = 0 is the necessary and sufficient condition for the factorization  $\rho_{AB} = \rho_A \otimes \rho_B$ , what means, of course, the absolute independence (non-correlativety) of A and B in the product state. Therefore, in the quantum information theory, one takes the mutual information to measure the total (both classical and quantum) correlations between the two subsystems of bipartite quantum system.

On the other hand, measurements performed on one system, in general, influence on the quantum state of another system (see, for instance,<sup>30</sup>). Postulating that the total classical part of correlations is the *maximal* amount of information about one subsystem, say A, that can be extracted by performing a measurement on the other subsystem B, Henderson and Vedral<sup>2</sup> suggested to take as a measure of classical correlation the quantity

$$C(\rho_{AB}) = \max_{\{B_i\}} \{ S(\rho_A) - \sum_i p_i S(\rho_A^i) \}.$$
 (8)

Here  $\{B_i\}$  is a complete set of measurements on the subsystem B,

$$\rho_A^i = \operatorname{Tr}_B(B_i \rho_{AB} B_i^+) / \operatorname{Tr}_{AB}(B_i \rho_{AB} B_i^+) \quad (9)$$

is the remaining state of A after obtaining the outcome i on B, and

$$p_i = \operatorname{Tr}_{AB}(B_i \rho_{AB} B_i^+) \tag{10}$$

is the probability to detect the result i.

Ollivier and Zurek<sup>3</sup>, on the contrary, focused their attention on an extraction of quantum correlations. Further analysis of the measurements led to the generalization of expression (4) for the quantum case,

$$I'(A:B) = S(\rho_A) - \sum_{i} p_i S(\rho_A^i).$$
 (11)

(It is obvious that the right hand of this equality is a non-optimized classical correlation of Henderson and Vedral.) In the paper<sup>3</sup>, the *minimal* difference  $I - I' \equiv Q$  has been identified with an amount of quantum correlation and has been called the quantum discord — a measure of the quantum excess of correlations, a measure of the quantumness of correlations. Taking into account that

$$I = C + Q, \tag{12}$$

we see the equivalentness of results of Henderson-Vedral and Ollivier-Zurek.

Quantum discord displays a number of properties (see, e. g., the reviews<sup>17,18</sup>). We note between them the following ones. For a pure state, discord coincides with the entanglement E. In mixed states, the quantum correlation (discord) can present even in that case when the entanglement is absent. Quantum discord  $Q \ge 0$ . Discord is limited from above by the entropy of one subsystem,  $Q \le S(\rho_{A(B)})$ . In particular, if the system is two-qubit and the logarithm base for entropy equals two then  $Q \le 1$ .

### III. HAMILTONIAN AND DENSITY MATRIX

Consider a system consisting of two identical particles with the spins 1/2 which couple between themselves by the magnetic dipole-dipole interaction. Let moreover, the external homogeneous magnetic field with induction **B** was applied to the system. Then the Hamiltonian of a model can be written as (see, e. g.,<sup>6</sup>)

$$\mathcal{H} = \mathcal{H}_{dd} + \mathcal{H}_Z, \tag{13}$$

where the dipolar part is

$$\mathcal{H}_{dd} = \frac{\mu_0}{4\pi} \frac{\gamma^2 \hbar^2}{4r^3} [\sigma_1 \sigma_2 - 3(\mathbf{n} \cdot \sigma_1)(\mathbf{n} \cdot \sigma_2)] \quad (14)$$

and the Zeeman energy equals

$$\mathcal{H}_Z = -\frac{1}{2}\gamma\hbar(\sigma_1 + \sigma_2)\mathbf{B}.$$
 (15)

In these equations,  $\mu_0$  is the magnetic constant (magnetic permeability of free space),  $\gamma$  is the gyromagnetic ratio,  $\sigma_{1,2}$  are the vectors of Pauli matrices at the sites 1 and 2, r is the distance between the spins in a dimer, **n** is the unit vector in the direction from one spin to the other, and **B** is the vector of magnetic field induction. The dipole-dipole interaction reflects the exact law (in that sense that it does not contain the fitting parameters), the interaction is sharply anisotropic and long-acting (in contrast, say, to the exchange interaction).

In the spherical coordinates when  $\mathbf{B} = (0, 0, B)$  and  $\mathbf{n} = (\sin \theta, 0, \cos \theta)$ , the Hamiltonian (13) - (15) takes the form

$$\mathcal{H} = \frac{\mu_0}{4\pi} \frac{\gamma^2 \hbar^2}{4r^3} [\sigma_1 \sigma_2 - 3(\sigma_1^x \sin \theta + \sigma_1^z \sin \theta) \\ \times (\sigma_2^x \sin \theta + \sigma_2^y \sin \theta)] - \frac{1}{2} \gamma \hbar B(\sigma_1^z + \sigma_2^z).$$
(16)

It has been shown<sup>31</sup> that when the polar angle  $\theta = \frac{\pi}{2}$  (the external field is applied perpendicularly to the direction of dimer longitudinal axis the entanglement in the system is maximal. On the contrary, when  $\theta = 0$  or  $\pi$  (the longitudinal dimer axis is parallel to the external field) the entanglement between spins is absent (below we prove this strongly/exactly).

Because the special interest is to discover and investigate the quantum correlations without entanglement, we will consider from this point the case  $\theta = 0$ . By this, the Hamiltonian (16) takes the form

$$\mathcal{H} = \frac{1}{2}D(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \Delta \sigma_1^z \sigma_2^z) - \frac{1}{2}h(\sigma_1^z + \sigma_2^z),$$
(17)

where the dipolar coupling constant equals

$$D = \frac{\mu_0}{4\pi} \frac{\gamma^2 \hbar^2}{2r^3} \tag{18}$$

and the normalized external field is

h

$$=\gamma\hbar B.$$
 (19)

In dipole-dipole coupled dimer, the anisotropy parameter is  $\Delta = -2$ . However, below we will, in some cases for the sake of generality, extend the values of  $\Delta$ . But all graphical and numerical material in our paper is presented for  $\Delta = -2$ .

The Hamiltonian (17) corresponds to the XXZ model in Z field. In the matrix forn, it

is given as

$$\mathcal{H} = \begin{pmatrix} \frac{\Delta}{2}D - h & & \\ & -\frac{\Delta}{2}D & D & \\ & D & -\frac{\Delta}{2}D & \\ & & & \frac{\Delta}{2}D + h \end{pmatrix}.$$
(20)

The  $2 \times 2$  subblock presented here is a centrosymmetric matrix which under the orthogonal transformation

$$O = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix} \tag{21}$$

undegoes in diagonal form.

The energy spectrum of the Hamiltonian (20) with condition  $\Delta = -2$  consists of two independent on external field levels

$$E_1 = 2D, \qquad E_2 = 0 \tag{22}$$

and two levels

$$E_{3,4} = -D \pm h.$$
 (23)

Because D > 0, the ground state energy is

$$E_0 = -D + |h|. (24)$$

In absence of external field, the ground state is two-fold degenerate.

We will consider the dimer in a termal equilibrium state. In this case, its density matrix  $\rho \equiv \rho_{AB}$  has the Gibbs form

$$\rho = \frac{1}{Z} \exp(-\beta \mathcal{H}), \qquad (25)$$

where  $\beta = 1/k_B T$ ,  $k_B$  is Boltzmann's constant, and Z is the partition function,

$$Z = \operatorname{Tr}\exp(-\beta\mathcal{H}). \tag{26}$$

Performing necessary calculations we find that in the original (standard) basis  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$  $|11\rangle$  the density matrix has the structure

$$\rho = \begin{pmatrix} a & & \\ & b & v \\ & v & b \\ & & & d \end{pmatrix},$$
(27)

where

$$a = \frac{1}{Z} \exp[-\beta(\frac{\Delta}{2}D - h)],$$
  

$$d = \frac{1}{Z} \exp[-\beta(\frac{\Delta}{2}D + h)],$$
  

$$b = \frac{1}{Z} \exp(\beta\frac{\Delta}{2}D) \operatorname{ch}\beta D,$$
  

$$v = -\frac{1}{Z} \exp(\beta\frac{\Delta}{2}D) \operatorname{sh}\beta D,$$
  
(28)

and partition function is

$$Z = 2(\operatorname{ch}\beta D + e^{-\beta D\Delta} \operatorname{ch}\beta h)e^{\beta D\Delta/2}.$$
 (29)

Expressions (28) satisfy the condition

$$a + d + 2b = 1,$$
 (30)

which provides the normalization  $Tr \rho = 1$ .

Expanding the density matrix (27) into powers of Pauli matrices we obtain it in the (normal) Bloch form

$$\rho = \frac{1}{4} [1 + (a - d)(\sigma_1^z + \sigma_2^z) + 2v(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + (1 - 4b)\sigma_1^z \sigma_2^z].$$
(31)

Expansion coefficients are the unary and binary correlators,

$$m \equiv \langle \sigma_1^z \rangle = \langle \sigma_1^z \rangle = a - d = \frac{2}{Z} e^{-\beta D \Delta/2} \mathrm{sh} \,\beta h,$$
(32)

$$G_{\parallel} \equiv \langle \sigma_1^z \sigma_2^z \rangle = 1 - 4b = 1 - \frac{4}{Z} e^{\beta D \Delta/2} \mathrm{ch} \,\beta D,$$
(33)

$$G_{\perp} \equiv \langle \sigma_1^x \sigma_2^x \rangle = \langle \sigma_1^y \sigma_2^y \rangle = 2v = -\frac{2}{Z} e^{\beta D \Delta/2} \mathrm{sh} \beta D$$
(34)

Brackets denote the trace operation for the expression in brackets with density operator,  $\langle \cdot \rangle = \text{Tr}(\cdot \rho)$ . The coefficient a - d = m in the expansion (31) is equal to the z components (projections) of the Bloch vectors for the reduced density matrices of subsystems A and B. Moreover, the quantities  $m, G_{\parallel}$ , and  $G_{\perp}$  have a physical sense, correspondingly, as the normalized magnetization, longitudinal and transverse components of correlation matrix. Relations

$$a = \frac{1}{4} (1 + 2m + G_{\parallel}), \qquad b = \frac{1}{4} (1 - G_{\parallel}),$$
$$v = \frac{1}{2} G_{\perp}, \qquad d = \frac{1}{4} (1 - 2m + G_{\parallel}) \quad (35)$$

give the expressions for the matrix elements of the density operator (27) through the system correlators.

From Eq. (32)–(34) we find the high temperature behavior for the magnetization and correlation functions,

$$m(T,h) = \frac{1}{2} \frac{h}{k_B T} - \frac{\Delta}{4} \frac{h}{D} \left(\frac{D}{k_B T}\right)^2 + O(1/T^3),$$
(36)
$$G_{\parallel}(T,h) = -\frac{\Delta}{2} \frac{D}{k_B T} - \frac{1}{4} \left[1 - \left(\frac{h}{D}\right)^2\right] \left(\frac{D}{k_B T}\right)^2$$

2

$$G_{\perp}(T,h) = -\frac{1}{2} \frac{D}{k_B T} - \frac{\Delta}{4} \left(\frac{D}{k_B T}\right)^2 + \frac{1}{8} \left[\frac{1}{3} + \left(\frac{h}{D}\right)^2\right] \left(\frac{D}{k_B T}\right)^3 + O\left(\frac{1}{T^4}\right).$$
(38)

Thus, when  $T \to \infty$ , the main contributions to the correlators tend to zero according to the law 1/T. By this, a weak external field does not exercise an influence on the  $G_{\parallel}$  and  $G_{\perp}$ . Moreover, the leading term in the expansion of the transverse correlator  $G_{\perp}$  does not depend on the anisotropy  $\Delta$ .

At lower temperature, the correlation functions for the dipolar dimer  $(D > 0, \Delta = -2)$  in absence of external field behave as

$$G_{\parallel}|_{T \to 0} \approx 1 - \exp(-\frac{D}{k_B T}), \qquad (39)$$

$$G_{\perp}|_{T \to 0} \approx -\frac{1}{2} \exp(-\frac{D}{k_B T}).$$
 (40)

If the field  $h \neq 0$ , the additional statistical weights at the exponents arise (due to a change of ground state of the system; see below),

$$G_{\parallel}|_{T \to 0} \approx 1 - 2 \exp(-\frac{D}{k_B T}), \qquad (41)$$

$$G_{\perp}|_{T \to 0} \approx -\exp(-\frac{D}{k_B T}).$$
 (42)

Thus, the lower temperature behavior of correlators is described by a function of the form  $e^{-1/x}$ .

#### IV. QUANTUM ENTANGLEMENT

The entanglement through the relation

$$E = -\frac{1 + \sqrt{1 - \tilde{C}^2}}{2} \log_2\left(\frac{1 + \sqrt{1 - \tilde{C}^2}}{2}\right) -\frac{1 - \sqrt{1 - \tilde{C}^2}}{2} \log_2\left(\frac{1 - \sqrt{1 - \tilde{C}^2}}{2}\right) \quad (43)$$

is expressed via the concurrence  $\tilde{C}^{32,33}$ .

In the case of density matrix having the block-diagonal form

$$\rho = \begin{pmatrix} u_1 & & \\ & x_1 & w & \\ & w^* & x_2 & \\ & & & u_2 \end{pmatrix},$$
(44)

the equation<sup>34</sup>

$$\tilde{C} = 2 \max\{|w| - \sqrt{u_1 u_2}, 0\}$$
 (45)

serves for calculation of concurrence. The expression (45) is a particular case of Hill-Wootters formula<sup>32,33</sup> which allows to calculate the pairwise concurrence in general two-qubit system.

Our density matrix (27) has the form of Eq. (44). Using Eqs. (28) we find that

$$|w| - \sqrt{u_1 u_2} = -v - \sqrt{ad} \le 0, \qquad (46)$$

if  $\Delta \leq -1$ . This inequality is valid for arbitrary external field *B*. Hence, the concurrence (45) and together with it the entanglement (43) are equal identically to zero. So, in the dipoledipole ( $\Delta = -2$ ) dimer under question, the quantum entanglement is absent for all temperatures and arbitrary longitudinal fields.

# V. INFORMATION CORRELATIONS

In this section, we give a calculation of information correlations in dipolar dimer both in and out magnetic field.

### A. Arbitrary external field

Discord in a system with the density matrix having the structure (27) equals<sup>35,36</sup>

$$Q = \min\{Q_1, Q_2\},$$
 (47)

where

$$Q_{1} = S_{A} - S_{AB} - a \log_{2} \left(\frac{a}{a+b}\right)$$
$$-b \log_{2} \left(\frac{b}{a+b}\right) - b \log_{2} \left(\frac{b}{b+d}\right)$$
$$-d \log_{2} \left(\frac{d}{b+d}\right), \qquad (48)$$

$$Q_2 = S_A - S_{AB} - \delta_1 \log_2 \delta_1 - \delta_2 \log_2 \delta_2, \quad (49)$$

and

$$\delta_{1,2} = \frac{1}{2} \left[ 1 \pm \left( (a-d)^2 + 4v^2 \right)^{1/2} \right].$$
 (50)

In equations (48) and (49),

$$S_A = -(a+b)\log_2(a+b) - (b+d)\log_2(b+d)$$
(51)

is the von Neumann entropy of reduced density matrix  $\rho_A$  and

$$S_{AB} = -a \log_2 a - d \log_2 d - (b+v) \log_2 (b+v) -(b-v) \log_2 (b-v)$$
(52)

equals the von Neumann entropy for the density matrix  $\rho$  of full system.

The total correlation is  $I = 2S_A - S_{AB}$ , and classical one C = I - Q. These relations and also (47)–(52) together with Eqs. (28) and (29) define the quantum discord, classical, and total correlations as functions of the temperature and external magnetic field by arbitrary values of parameters D and  $\Delta$ .

At high temperatures,

$$Q_{1} = \frac{1}{4\ln 2} \left(\frac{D}{k_{B}T}\right)^{2} + \frac{\Delta}{8\ln 2} \left(\frac{D}{k_{B}T}\right)^{3} + O(1/T^{4}),$$
(53)
$$Q_{2} = \frac{1}{4\ln 2} \left(1 + \Delta^{2}\right) \left(\frac{D}{2}\right)^{2} + O(1/T^{3}),$$
(54)

$$Q_2 = \frac{1}{8\ln 2} \left(1 + \Delta^2\right) \left(\frac{D}{k_B T}\right)^2 + O(1/T^3).$$
 (54)

Thus, the main terms of these expressions do not depend on the external magnetic field. From the relations (53) and (54), one can see that by  $|\Delta| > 1$  the discord, according to Eq. (47), is defined by the branch  $Q_1$ . Hence, when  $\Delta > 1$  or  $\Delta < -1$ , the quantum discord by high temperatures behaves as

$$Q|_{T \to \infty} \approx \frac{1}{4 \ln 2} \frac{1}{(k_B T/D)^2}.$$
 (55)

Thus, it does not depend on both external magnetic field or interaction anisotropy  $\Delta$ . With increasing the temperature, the quantum correlations decrease according to the law  $1/T^2$ , i. e., essentially rapidly than ordinary statistical correlations which, how it can was emphasized above, tend to zero according to the law 1/T.

From equations presented above, we establish also that by high temperatures the classical correlation is

$$C|_{T \to \infty} \approx \frac{\Delta^2}{8\ln 2} \frac{1}{(k_B T/D)^2} \tag{56}$$

and does not depend on external field.

### B. Dimer in absence of external field

In important particular case of zero external field, the information correlations can be calculated via the simpler formulas<sup>37</sup>. In absence of



Figure 1: Quantum discord in dipolar system  $(\Delta = -2)$  as a function of temperature and external longitudinal magnetic field.

field, a = d and  $S_A = S_B = 1$ . Besides, using expressions (33) and (34), it is not difficult to establish that by  $\Delta < -1$  one has  $G_{\parallel} \ge |G_{\perp}|$ (below this will be seen in graphics). Therefore, in absence of magnetic field, the classical part of mutual correlations is

$$C = \frac{1}{2} \left[ (1+G_{\parallel}|) \log_2(1+G_{\parallel}|) + (1-G_{\parallel}|) \log_2(1-G_{\parallel}|) \right]$$
(57)

and the quantum discord equals

1

$$Q = \frac{1}{4} \left[ (1 + 2G_{\perp} - G_{\parallel}) \log_2(1 + 2G_{\perp} - G_{\parallel}) - 2(1 - G_{\parallel}) \log_2(1 - G_{\parallel}) + (1 - 2G_{\perp} - G_{\parallel}) \cdot \log_2(1 - 2G_{\perp} - G_{\parallel}) \right].$$
(58)

How can one see from Eq. (57), the classical correlation is completely determined by the longitudinal correlator  $G_{\parallel}$ . Using expressions for the correlation functions (33), (34) and setting h = 0 in them, we get the following formula for the discord,

$$Q(T) = \frac{\frac{D}{k_B T} \operatorname{sh} \frac{D}{k_B T} - \operatorname{ch} \frac{D}{k_B T} \ln[\operatorname{ch} \frac{D}{k_B T}]}{(\operatorname{ch}(\frac{D}{k_B T}) + \exp(-\frac{D\Delta}{k_B T})) \ln(2)}.$$
(59)

For a dipolar dimer  $(D > 0, \Delta = -2)$  in zero field and at lower temperatures, we have

$$Q|_{T\to 0} \approx \frac{1}{2} \exp\left(-D/k_B T\right). \tag{60}$$

Arbitrary order derivatives with respect to the temperature for the function in the right hand of this equation is zero at T = 0. Therefore, by small deviation of temperature from absolute zero,  $Q \approx 0$ . This is connected with existence of a gap in the energy spectrum of the system.



Figure 2: Isolines of quantum discord in dipolar system ( $\Delta = -2$ ).

### VI. DISCUSSION

A behaviour of quantum discord in the dipole-dipole system under question ( $\Delta = -2$ ) is shown in Fig. 1. We see the smooth hill-like surface stretched in the temperature axis direction. Along a straight line h = 0, two ridges go; one ridge goes in the direction of temperature decreasing and the other in the direction of its increasing. The surface is symmetrical under reflection in vertical plane going through the hill top and the straight line h = 0 in the temperature-field plane. By given temperature, the discord is maximal in absence of external magnetic field, that is, the field leads only to a suppression of quantum correlation. At the absolute zero temperature, the discord in dimer is identically equal to zero. In the high temperature limit, quantum correlation is also vanished. In Fig. 2, the cross sections (profiles) of a discord surface are shown by different values of Q. It is seen that the isolines form a set of noncrossing ovals.

To study in detail the behavior of discord, we represented in VI its temperature dependence by different values of external field. The discord reaches the largest value at h = 0 and

$$k_B T_m / D = 0.881\,297\dots$$
 (61)

The discord in this point equals

$$Q_m = 0.083\,061\dots$$
 (62)

what is 8.3% of maximal value which is possible in any two-qubit system. The value (61), we have found both by a numerical search of maximum for the function Q of  $k_BT/D$  and from



Figure 3: Discord isoterms by different values of external field.

solution of transcendental equation

 $x(e^{\Delta \cdot x} + \operatorname{ch} x + \Delta \cdot \operatorname{sh} x) = (\operatorname{sh} x + \Delta \cdot \operatorname{ch} x) \ln(\operatorname{ch} x),$ (63)

where  $x = D/k_BT$ . This equation follows from the condition  $\partial Q/\partial T = 0$  in which the function Q(T) is given by expression (59).

One can see from Fig. 3 that, with increasing the field, the discord maximum is moved in the direction of higher temperatures. This is a good feature. However by this the value of discord at the maximum is less than its value at the same temperature in absence of external field.

We see also that with the help of external field and temperature (these parameters are in our hands), one can control the discord varying its value from zero to 0.083 bit per a dimer.

Let us consider the case when the dipolar dimer is in absence of external field. The temperature dependences of ordinary spin-spin correlation functions  $G_{\parallel}$  and  $|G_{\perp}|$  ( $G_{\perp} \leq 0$ , therefore its absolute value is taken), as well as total classical correlation C and discord Q are presented in Fig. 4. At zero temperature, both longitudinal and total classical correlation are equal to their maximal magnitudes. The temperature increasing leads only to their decrease. Both the value of transverse correlation  $|G_{\perp}|$ and quantum discord are zero at T = 0.

To clarify the situation in correlation behavior at zero, we consider the limit of density matrix (27) when  $T \rightarrow 0$ . Using the expressions



Figure 4: Temperature behavior of statistical  $(G_{\parallel})$  and  $|G_{\perp}|$ , classical (C), and quantum (Q) correlations in absence of magnetic field.

for its matrix elements (28) one finds

$$\rho|_{T=0} = \begin{pmatrix} 1/2 & & \\ & 0 & \\ & & 0 \\ & & & 1/2 \end{pmatrix}.$$
 (64)

This matrix has the expansion

$$\rho = \frac{1}{2} (|0\rangle \langle 0|_A \otimes |0\rangle \langle 0|_B + |1\rangle \langle 1|_A \otimes |1\rangle \langle 1|_B, \ (65)$$

i. e., it is a sum of the direct products of separate particles. Such state belongs to the class of purely classical ones<sup>38</sup> and therefore, according to the criteria<sup>39</sup>, all quantum correlations in it are entirely absent. This explains that we obtained  $Q|_{T=0} = 0$ . On the other hand, classical correlations are available and equal the total correlations C = I.

So the behavior of system at T = 0 is purely classical. However, with increasing the temperature, the behavior acquires the quantum features, i. e., the temperature leads to the generation of quantum correlations. Such unusual phenomenon (it is much ordinary when the temperature destroys the quantum states) one can explain by following. In the Hamiltonian (17) with  $\Delta < -1$ , the purely classical ferromagnetic contribution

$$H_{zz} = \Delta D \sigma_1^z \sigma_2^z \tag{66}$$

is dominate at lower temperatures. The transverse components of spins are actually "frozen" CORRELATIONS



Figure 5: The same as in Fig. 4 but in presence of a field.

(the value  $G_{\perp} = 0$  witnesses this). With increasing the temperature these degrees of freedom "revive" and the system from classical becomes a quantum one. But when the temperature fluctuations begin to exceed the system energy gap, the temperature produces its usual destroying action and the correlations go down to non.

From Fig. 4 and asymptotical behavior of correlations, it is not difficult to notice a correspondence in qualitative behavior, on the one hand, C and  $G_{\parallel}^2$  and, on the other hand, Q and  $G_{\perp}^2$ . The latter correspondence is not an accident. Indeed, if the quantum correlation is measured by geometrical discord  $Q_g$ , i. e., by a distance (in sense of the Hilbert-Schmidt norm) from the given state  $\rho$  to the nearest classical one, the general formula<sup>39,40</sup> applied to the density matrix (31) by an absence of external field yields

$$Q_g = G_\perp^2. \tag{67}$$

Consider now the situation in a presence of external magnetic field. In Fig. 5, the behavior of different correlations is again shown but for h/D = 0.1. It is seen that correlations  $G_{\parallel}, G_{\perp}$ , and Q were changed weakly. But the behavior of classical correlation C undergoes an essential change — it tends now to zero when  $T \rightarrow 0$ . At the point of absolute zero temperature, there are no any correlations in the system at all.

To understand a happening, we turn out again to the density matrix. The matrix (27)



Figure 6: Classical correlation vesus the field by diffrrent values of temperature.

in the limit  $T \to 0$  is equal now to both

$$\rho|_{T=0} = \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \\ & & & 0 \end{pmatrix}, \quad (68)$$

if h > 0 or

$$\rho|_{T=0} = \begin{pmatrix} 0 & & \\ & 0 & \\ & & 0 & \\ & & & 1 \end{pmatrix},$$
 (69)

if h < 0. These states correspond to the completely orderings of spins along the field. Both matrices (68) and (69) are factorized into a direct product of two density matrices  $2 \times 2$ ,

$$\begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$
$$\begin{pmatrix} 0 & & \\ & 0 & \\ & & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} (70)$$

This means that the states (68) and (69) are completely uncorrelated and therefore any correlations are absent in them.

Emphasize that  $G_{\parallel} \neq 0$  at T = 0 does not contradict to the said above. In the factorized state must be zero only the centered correlator. By  $h \neq 0$ , the spins at the point of absolute zero temperature are ordered and therefore

$$\langle (\sigma_1^z - \langle \sigma_1^z \rangle) (\sigma_2^z - \langle \sigma_2^z \rangle) \rangle = 0.$$
 (71)

Thus, any statistical relation between spins is also absent.

Fig. 6 shows the behavior of classical correlation C upon the external field. The curves have the form of bell-like splashes. Their largest value is arrived at in the point when the field vanishes. With decreasing the temperature, the maximums become more narrow and their value tends to the value C = 1. At T = 0, a splash becomes infinitely thin,

$$C = \begin{cases} 1, & h = 0\\ 0, & h \neq 0 \end{cases}.$$
 (72)

The external field sweeping will on a moment lead to a spasmodic jump appearance of classical correlation and at the same time to a disappearance of this correlation by going the field of the zero point. By this, the quantum correlation in the system does not arise.

Let's turn to the available experimental data. Measurements performed by the nuclear magnetic resonance (NMR) at room temperature show that in gypsum crystals  $CaSO_4 \cdot 2H_2O$ the distance between protons in each water molecule is  $r = 0.158 \text{ nm}^{21}$  (see also, e. g., the book $^{23}$ ). For protons, the gyromagnetic ratio, as it is known<sup>24</sup>, equals  $\gamma = 2.675$ .  $10^8 \text{ rad/(c·T)}$ , therefore the dipole-dipole coupling constant (18) in gypsum is  $D/k_B =$  $0.73 \ \mu K$  (in temperature units). Consequently, in accord with (61), the maximum discord value  $Q_{max} = 0.083$  will arrive at the temperature 0.64  $\mu$ K. At room temperature (T = 300), the discord in gypsum, according to (55), must be equal to  $Q \sim 2 \cdot 10^{-18}$ . In spite of extremely small value of quantum correlations in spin-nuclear systems at room temperatures, at present the attempts are undertaken to detect their by NMR methods  $^{41-44}$ .

As an another example, let us consider 1,2dichloroethane  $\text{ClH}_2\text{C} - \text{CH}_2\text{Cl}$ . In this compound, two protons at each carbon atoms are coupled much stronger between themselves by dipole-dipole interaction than with protons belong to an other carbon atom. NMR measurements performed on solid dichloroethane at the temperature 90 K have shown that here  $r = 0.17(2) \text{ nm}^{22}$  (see  $\text{also}^{23,24}$ ). Using again the relations (18) and (61), we estimate the temperature for the discord maximum in this substance as  $T_m = 0.517 \ \mu\text{K}$ . At the temperature 90 K, the value of quantum correlations must equal  $Q \sim 1.5 \cdot 10^{-17}$ .

### VII. CONCLUSIONS

In the paper, a study of information correlations in dipolar dimers both in absence of external magnetic field and in the field directed along the longitudinal axis of a dimer has been performed. It has been shown that the quantum correlations are completely absent at the absolute zero temperature and arbitrary strength of magnetic field but they arise with increasing the temperature. We proposed an interpretation such of phenomenon.

In the high temperature region, the discord obeys the law

$$Q \sim G_{\perp}^2 \sim 1/(k_B T/D)^2$$
.

This, in particular, means that at room, nitrogen, or helium temperatures, the non-zero quantities of spin-spin correlations between the xx or yy spin components can serve as a witness of quantum correlations. The spin-spin correlations go down with increasing the temperature according to the essentially slow law  $T^{-1}$  and one can directly measure them, for example, in scattering experiments.

It was shown also that the classical correlations have a sharp maximum in the point of zero external magnetic field when  $T \rightarrow 0$ .

A qualitative analogy between the quantum discord and the squared correlator  $G_{\perp}$  has been found. In supporting this observation, it was shown that the geometrical discord equals  $Q_g = G_{\perp}^2$ .

In the paper, the estimates for the thermal quantum discord between spins of hydrogen nucleous  ${}^{1}\text{H}$  in gypsum and 1,2-dichloroethane have been done.

Our investigation can be extended to manynuclear clusters if to perform a density matrix reduction for all spins except any two. Experimental NMR data are available for clusters in a form, for example, triangles, tetrahedron, linear magnetic structures, etc.,<sup>23,45,46</sup>.

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- <sup>1</sup> W. H. Zurek, Ann. Phys. (Leipzig) **9**, 855 (2000).
- <sup>2</sup> L. Henderson and V. Vedral, J. Phys. A: Math. Gen. **34**, 6899 (2001).
- <sup>3</sup> H. Ollivier and W. H. Zurek, Phys. Rev. Lett. 88, 017901 (2002).
- <sup>4</sup> V. Vedral, Phys. Rev. Lett. **90**, 050401 (2003).
- <sup>5</sup> W. H. Zurek, Phys. Rev. A **67**, 012320 (2003).
- <sup>6</sup> M. A. Nielsen and I. L. Chung, *Quantum Computation and Quantum Information* (Cambridge Universaty Press, Cambridge, 2000).
- <sup>7</sup> K. A. Valiev and A. A. Kokin, *Quantum Computers: Hops and Reality* (Reseach Center "Regular and Chaotic Dynamics", Moscow and Izhevsk, 2002) (in Russian).
- <sup>8</sup> K. A. Valiev, Usp. Fiz. Nauk **175**, 3 (2005) [Phys.—Usp. **48** 1 (2005)].
- <sup>9</sup> L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
- <sup>10</sup> R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. **81**, 865 (2009).
- <sup>11</sup> A. Datta, A. Shaji, and C. M. Caves, Phys. Rev. Lett. **100**, 050502 (2008).
- <sup>12</sup> B. P. Lanyon, M. Barbieri, M. P. Almeida, and A. G. White, Phys. Rev. Lett. **101**, 200501 (2008).
- <sup>13</sup> R. Dillenschneider, Phys. Rev. B 78, 224413 (2008).

- <sup>14</sup> M. S. Sarandy, Phys. Rev. A **80**, 022108 (2009).
- <sup>15</sup> T. Werlang, C. Trippe, G. A. P. Ribeiro, and G. Rigolin, Phys. Rev. Lett. **105**, 095702 (2010).
- <sup>16</sup> A. Ferraro, L. Aolita, D. Cavalcanti, F. M. Cucchietti, and A. Acín, Phys. Rev. A **81**, 052318 (2010).
- <sup>17</sup> L. C. Céleri, J. Maziero, and R. M. Serra, Int. J. Quant. Inf. 9, 1837 (2011).
- <sup>18</sup> K. Modi, A. Brodutch, H. Cable, T. Paterik, and V. Vedral, Rev. Mod. Phys. **84**, 1655 (2012).
- <sup>19</sup> G. R. Khutsishvili, Usp. Fiz. Nauk **40**, 621 (1950).
- <sup>20</sup> J. Jensen and A. R. Mackintosh, *Rare Earth Magnetism. Structures and Excitations*, (Clarendon Press, Oxford, 1991).
- <sup>21</sup> G. E. Pake, J. Chem. Phys. **16**, 327 (1948).
- <sup>22</sup> H. S. Gutowsky, G. B. Kistiakowsky, G. E. Pake, and E. M. Purcell, J. Chem. Phys. **17**, 972 (1949).
- <sup>23</sup> A. Abragam, The Principles of Nuclear Magnetism, (Clarendon Press, Oxford, 1961).
- <sup>24</sup> H. Günter, NMR Spectroskopy. An introduction, (Wiley, Chichester, New York, Brisbane, Toronto, 1980).
- <sup>25</sup> G. A. Korn and T. M. Korn, Mathematical Handbook for Scientists and Engineers, (McGraw-Hill Book, 1968).
- <sup>26</sup> V. P. Chistyakov, *Course of Probability Theory*, (Nauka, Moscow, 1982) (in Russian).

- <sup>27</sup> V. V. Mityugov, *Physical Principles of Informa*tion Theory, (Soviet Radio, Moscow, 1976) (in Russian).
- <sup>28</sup> T. M. Cover and J. A. Thomas, *Elements of Information Theory*, (Wiley, New York, 1991).
- <sup>29</sup> A. S. Holevo, *Quantum Systems, Channels, Information*, (MTsNMO, Moscow, 2010) (in Russian).
- <sup>30</sup> A. S. Holevo, Probability and Statistical Aspects of Quantum Theory, (MTsNMO, Moscow, 2003).
- <sup>31</sup> G. B. Furman, V. M. Meerovich, and V. L. Sokolovsky, Quant. Inf. Process. **10**, 307 (2011).
- <sup>32</sup> S. Hill and W. K. Wootters, Phys. Rev. Lett. 78, 5022 (1997).
- <sup>33</sup> W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
- <sup>34</sup> K. M. O'Connor and W. K. Wootters, Phys. Rev. A **63**, 052302 (2002).
- <sup>35</sup> F. F. Fanchini, T. Werlang, C. A. Brasil, L. G. E. Arruda, and A. O. Caldeira, Phys. Rev. A 81, 052107 (2010).
- <sup>36</sup> B. Li, Z.-X. Wang, and S.-M. Fei, Phys. Rev. A 83, 022321 (2011).
- <sup>37</sup> S. Luo, Phys. Rev. A **77**, 042303 (2008).
- <sup>38</sup> T. Paterek, W. Son, V. Vedral, and

M. Williamson, Phys. Rev. Lett. **104**, 080501 (2010).

- <sup>39</sup> B. Dakić, V. Vedral, and Č. Brukner, Phys. Rev. Lett. **105**, 190502 (2010).
- <sup>40</sup> B. Dakić, Y. O. Lipp, X. Ma, M. Ringbauer, S. Kropatschek, S. Barz, T. Paterek, V. Vedral, A. Zeilinger, C. Brukner, and P. Walther, arXiv:1203.1629v1 [quant-ph].
- <sup>41</sup> R. Auccaise, J. Maziero, L. C. Celeri, D. O. Soares-Pinto, E. R. deAzevedo, T. J. Bonagamba, R. S. Sarthour, I. S. Oliveira, and R. M. Serra, Phys. Rev. Lett. **107**, 070501 (2011).
- <sup>42</sup> J. Maziero, R. Auccaise, L. C. Celeri, D. O. Soares-Pinto, E. R. deAzevedo, T. J. Bonagamba, R. S. Sarthour, I. S. Oliveira, and R. M. Serra, arXiv:1212.2427v1 [quant-ph].
- <sup>43</sup> G. Passante, O. Moussa, D. A. Trottier, and R. Laflamme, Phys. Rev. A 84, 044302 (2011).
- <sup>44</sup> H. Katiyar, S. S. Roy, T. S. Mahesh, and A. Patel, Phys. Rev. A 86, 012309 (2012).
- <sup>45</sup> N. M. Alexandrov and F. I. Skripov, Usp. Fiz. Nauk **75**, 585 (1961).
- <sup>46</sup> J. Zhang, M. Ditty, D. Burgarth et al., Phys. Rev. A 80, 012316 (2009).